

Scattering in tight atom waveguides

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Abstract

Using the Theory of Scattering in Restricted Geometries developed by A. Lupu-Sax as a starting point, we present a comprehensive multi-channel theory of atom-atom scattering in tight atom waveguides.

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Conventions and notations

Square root conventions

Throughout the text we will be using two complementary conventions for the complex square root function: the usual convention \sqrt{z} defined as

$$\sqrt{|z|e^{i\phi}} = \sqrt{|z|}e^{i\phi/2} \quad 0 \leq \phi < 2\pi \quad ,$$

and a non-traditional $\sqrt[4]{z}$ one defined as

$$\sqrt[4]{|z|e^{i\phi}} = \sqrt{|z|}e^{i\phi/2} \quad -2\pi < \phi \leq 0 \quad .$$

Some notations

$\hat{G}_{\hat{H}}(E)$	Green's function of a Hamiltonian \hat{H}
$\hat{T}_{\hat{H},\hat{V}}(E)$	T-matrix of a perturbation \hat{V} to a Hamiltonian \hat{H}
$\hat{G}(E)$	Green's function of the harmonic waveguide with no scatterer present
$\chi_{\hat{H}}(E)$	regular part of the Green's function of a Hamiltonian \hat{H} at the origin
$\chi(E)$	regular part of the harmonic waveguide Green's function at the origin
$\mathcal{E} = E/2\hbar\omega_{\perp} - 1/2$	rescaled and renormalized energy
$a_{\perp} = \sqrt{\hbar/\mu\omega_{\perp}}$	transverse harmonic oscillator length
$ nm\rangle$	eigenstates of the two-dimensional harmonic oscillator
a	three-dimensional scattering length
$g = 2\pi\hbar^2 a/\mu$	three-dimensional coupling constant
a_{1D}	one-dimensional scattering length
$g_{1D} = -\hbar^2/\mu a_{1D}$	one-dimensional coupling constant

1 INTRODUCTION

Atom waveguides are a fundamental component of Atom Optics, and are expected to play an important role in Atom Interferometry and Quantum Computing applications. To ensure proper coherence as atomic beams propagate through the waveguides, effort should be made to avoid decoherence-inducing mechanisms such as collisional losses and collisional phase shifts. This clearly requires a detailed understanding of the effects of quasi-one-dimensional confinement on atom-atom collisions. In particular, we will see that in the few-mode regime, necessary for coherent propagation, the free-space estimates of the collisional effects are no longer valid and a waveguide-specific theory is needed.

Such one-dimensional interacting atomic quantum gases have recently been attracting significant theoretical and experimental interest, having become accessible via adiabatic transfer from atomic Bose condensates to highly elongated tight cigar-shape traps. Here the question of *effective one-dimensional coupling constants* becomes important, as they play a crucial role in determining whether or not the ground state possesses long-range order (coherence). In the regime of tight confinement it is the virtual excitation of the transverse modes which play a crucial role, leading to the confinement-induced renormalization of interatomic interactions [1, 2] (see

also the two-dimensional analog of such a renormalization described in [3] and the fermionic p-wave analog in [4]).

In this paper we present a comprehensive theory of atom-atom scattering in atom waveguides. Our theory correctly takes into account both quantization of the transverse motion and the transverse renormalization of the collisional strength, otherwise inaccessible by the free-space scattering theory.

From the formal point of view the problem reduces to a Schrödinger equation for two atoms in a harmonic waveguide. In this paper we concentrate on the universal properties of the waveguide scattering which are governed uniquely by the scattering length. The Theory of Scattering in Restricted Geometries developed by A. Lupu-Sax [5] allows us to describe these properties without invoking the full interaction potential, which is very often unknown.

2 FORMULATION OF THE SCATTERING PROBLEM

We begin from the Hamiltonian for two atoms under transverse harmonic confinement and subject to an arbitrary interaction potential

$$\begin{aligned}\hat{H}_2 &= -\frac{\hbar^2}{2m_1}\nabla_1^2 - \frac{\hbar^2}{2m_2}\nabla_2^2 + \frac{1}{2}m_1\omega_\perp^2\mathbf{r}_{1\perp}^2 + \frac{1}{2}m_2\omega_\perp^2\mathbf{r}_{2\perp}^2 \\ &+ V(\mathbf{r}_1 - \mathbf{r}_2)\end{aligned}\quad (2.1)$$

where m_1 and m_2 are the atomic masses, ω_\perp is the transverse trap frequency, and ∇_i^2 and $\mathbf{r}_{i\perp}$ are the Laplacian and radial coordinate of the i^{th} atom, respectively. This Hamiltonian is separable in relative and center-of-mass coordinates $\mathbf{R} = (m_1\mathbf{r}_1 + m_2\mathbf{r}_2)/M$, $\mathbf{r} = \mathbf{r}_1 - \mathbf{r}_2$, $M = m_1 + m_2$ being the total mass, yielding $\hat{H}_2 = \hat{H}_{rel} + \hat{H}_{COM}$, where

$$\hat{H}_{rel} = -\frac{\hbar^2}{2\mu}\nabla_{\mathbf{r}}^2 + \frac{1}{2}\mu\omega_\perp^2\mathbf{r}_\perp^2 + V(\mathbf{r}), \quad (2.2)$$

and

$$\hat{H}_{COM} = -\frac{\hbar^2}{2M}\nabla_{\mathbf{R}}^2 + \frac{1}{2}M\omega_\perp^2\mathbf{R}_\perp^2, \quad (2.3)$$

where $\mu = m_1m_2/(m_1 + m_2)$ is the reduced mass, and \mathbf{r}_\perp and \mathbf{R}_\perp are the relative and center-of-mass radial coordinates, respectively. The center-of-mass Hamiltonian is that of a simple harmonic oscillator whose solution is known, hence we focus only on the relative motion of the two particles. This reduces the problem to a single particle of mass μ , subject to transverse harmonic confinement, which is scattered by an external potential $V(\mathbf{r})$. The central equation which must be solved is therefore Schrödinger's equation for the state of relative motion of the two atoms

$$\left[E - \hat{H} - \hat{V}\right]|\psi(E)\rangle = 0 \quad (2.4)$$

where $\hat{H} = \hat{H}_{rel}$ and \hat{V} is the interatomic potential. Determining the eigenstates of this Hamiltonian, in particular within the s-wave scattering approximation for $V(\mathbf{r})$, is the central goal of this paper.

3 GREEN'S FUNCTION AND T-MATRIX FORMALISM

3.1 Definitions and theorems

In this section briefly review the T-matrix formulation of scattering theory, which provides a convenient framework for approaching the present problem. Let us first introduce the retarded

Green's function for a system with the Hamiltonian \hat{H} and energy E

$$\hat{G}_{\hat{H}}(E) = \lim_{\epsilon \rightarrow 0^+} (E + i\epsilon - \hat{H})^{-1}. \quad (3.1)$$

We then define the T-matrix at energy E of the scatter \hat{V} in the presence of the background Hamiltonian \hat{H} (Fig.1a,b) in the usual manner as

$$\begin{aligned} \hat{T}_{\hat{H},\hat{V}}(E) &= \left[1 - \hat{V} \hat{G}_{\hat{H}}(E) \right]^{-1} \hat{V} \\ &= \sum_{n=0}^{\infty} \left[\hat{V} \hat{G}_{\hat{H}}(E) \right]^n \hat{V}, \end{aligned} \quad (3.2)$$

the summation form being valid provided that there are no difficulties with convergence.

Two relations on which we will rely heavily are the Lippman-Schwinger relation

$$\hat{G}_{\hat{H}+\hat{V}}(E) = \hat{G}_{\hat{H}}(E) + \hat{G}_{\hat{H}}(E) \hat{T}_{\hat{H},\hat{V}}(E) \hat{G}_{\hat{H}}(E), \quad (3.3)$$

which relates the full Green's function of the system $\hat{H} + \hat{V}$ to the unperturbed Green's function $\hat{G}_{\hat{H}}(E)$ and the T-matrix, and the Lippman-Schwinger formula (Fig.1c)

$$\hat{T}_{\hat{H},\hat{V}}(E) = \left[1 - \hat{T}_{\hat{H}',\hat{V}}(E) \left[\hat{G}_{\hat{H}}(E) - \hat{G}_{\hat{H}'}(E) \right] \right]^{-1} \hat{T}_{\hat{H}',\hat{V}}(E), \quad (3.4)$$

which relates the T-matrix of the scatter \hat{V} in the background Hamiltonian \hat{H} (Fig.1b) to the T-matrix for the same scatter but in a different background Hamiltonian \hat{H}' (Fig.1a). Derivations for these expressions are given in Appendices B.2 and B.3, respectively.

3.2 Scattering theory

In the continuous part of the spectrum of the total Hamiltonian $\hat{H} + \hat{V}$ its eigenstates can be expressed as a sum of an incident and a scattered wave according to

$$|\psi(E)\rangle = |\psi_0(E)\rangle + |\psi_s(E)\rangle, \quad (3.5)$$

where $|\psi_0(E)\rangle$, the 'incident' state vector, satisfies

$$\hat{G}_{\hat{H}}^{-1}(E) |\psi_0(E)\rangle = 0, \quad (3.6)$$

we can then express the Schrödinger equation for the total system as

$$\left[\hat{G}_{\hat{H}}^{-1}(E) - \hat{V} \right] (|\psi_0(E)\rangle + |\psi_s(E)\rangle) = 0. \quad (3.7)$$

This equation is readily solved for the scattered wave in terms of the unperturbed Green's function and the T-matrix (see Appendix B.1), yielding

$$|\psi_s(E)\rangle = \hat{G}_{\hat{H}}(E) \hat{T}_{\hat{H},\hat{V}}(E) |\psi_0(E)\rangle, \quad (3.8)$$

which will serve as the basis for our treatment of the present scattering problem.

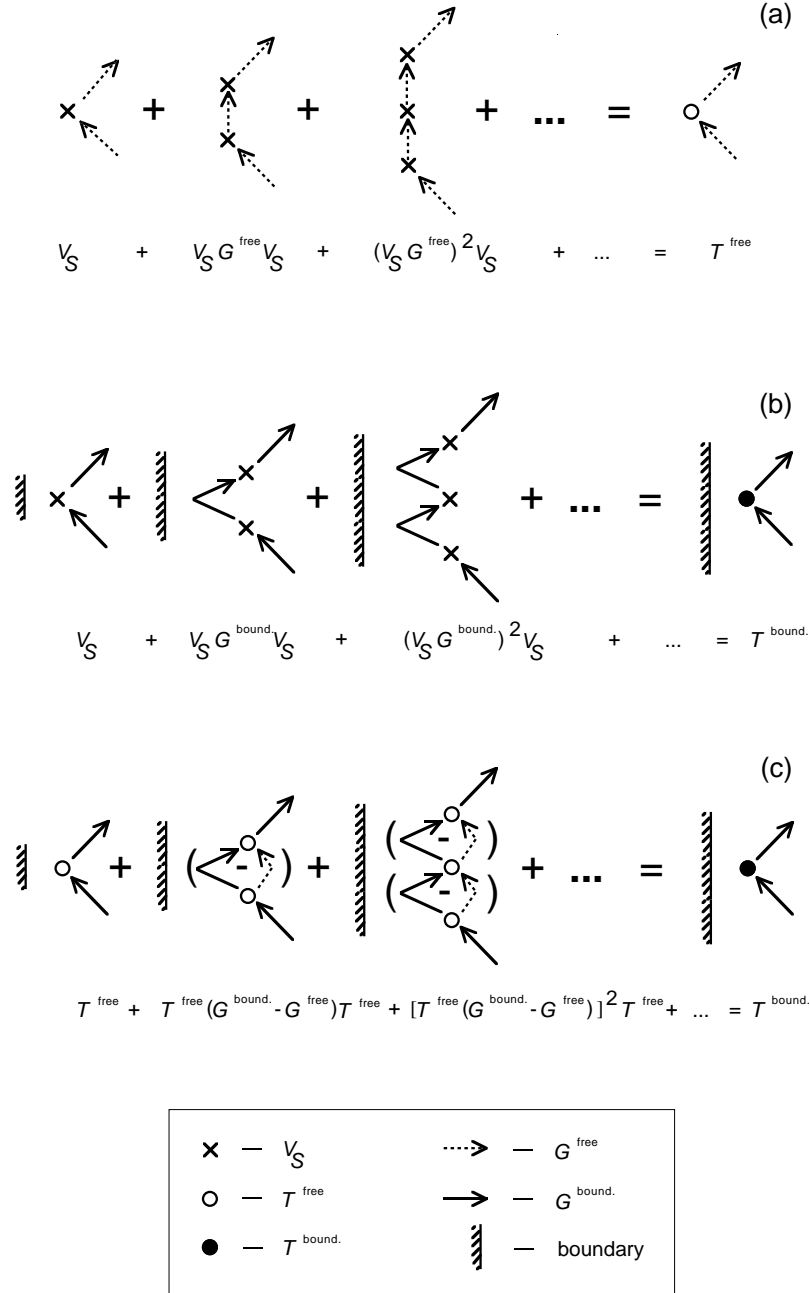


Fig. 1. An artist view on the Lupu-Sax theorem. Here $G^{\text{free}} = \hat{G}_{\hat{H}_0}(E)$, $G^{\text{bound.}} = \hat{G}_{\hat{H}_0 + \hat{U}^{\text{bound.}}}(E)$, $T^{\text{free}} = \hat{T}_{\hat{H}_0, \hat{V}_s}(E)$, $T^{\text{bound.}} = \hat{T}_{\hat{H}_0 + \hat{U}^{\text{bound.}}, \hat{V}_s}(E)$. In our problem \hat{H}_0 corresponds to the kinetic energy, $\hat{U}^{\text{bound.}}$ is the waveguide potential, and \hat{V}_s is the interatomic interaction potential.

3.3 Bound T-matrix as a generator for bound state energies

It follows from Eq. (3.1) that $\hat{G}_{\hat{H}}(E)$ is diagonal in energy representation and therefore takes the form

$$\hat{G}_{\hat{H}}(E) = \sum_n \frac{|E_n\rangle\langle E_n|}{E - E_n} + \sum_j \int_{E_{l,j}}^{E_{u,j}} dE' \frac{|E', j\rangle\langle E', j|}{E - E' + i\epsilon}, \quad (3.9)$$

where the first term on the r.h.s. sums over the discrete portion of the spectrum of \hat{H} and the second term sums over all continuous bands of the spectrum. The limit $\epsilon \rightarrow 0^+$ is implied. From this expression we see that in the discrete (bound-state) part of the spectrum the poles of the Green's function correspond to the bound state energies.

Consider now the particular case where the background Green's function $\hat{G}_{\hat{H}}(E)$ has only a continuous spectrum bounded from below by $E = 0$, i.e.

$$\hat{G}_{\hat{H}}(E) = \int_0^\infty dE' \frac{|E'\rangle\langle E'|}{E - E' + i\epsilon}. \quad (3.10)$$

Now consider a system consisting of this background Hamiltonian \hat{H} plus a scattering potential \hat{V} , described by the T-matrix $\hat{T}_{\hat{H}, \hat{V}}(E)$. Inserting equation (3.10) into the Lippman-Schwinger Equation (3.3) for the total Green's function gives

$$\hat{G}_{\hat{H}+\hat{V}}(E) = \int_0^\infty dE' \frac{|E'\rangle\langle E'|}{E - E' + i\epsilon} + \int_0^\infty \int_0^\infty dE' dE'' \frac{|E'\rangle\langle E'| \hat{T}_{\hat{H}, \hat{V}}(E) |E''\rangle\langle E''|}{(E - E' + i\epsilon)(E - E'' + i\epsilon)} \quad (3.11)$$

If a bound state of the combined system $\hat{H} + \hat{V}$ having energy $E_n < 0$ exists, then the full Green's function must take the form

$$\hat{G}_{\hat{H}+\hat{V}}(E) \stackrel{E \approx E_n}{\approx} \frac{|E_n\rangle\langle E_n|}{E - E_n}. \quad (3.12)$$

Since the background Green's function has no pole at E_n , it follows that the T-matrix itself must have a singularity at $E = E_n$. Finding the poles of the T-matrix below the lower bound of the spectrum of the background Hamiltonian therefore gives a method for determining the bound state energies of the system $\hat{H} + \hat{V}$.

4 S-WAVE SCATTERING REGIME: THE REFERENCE T-MATRIX APPROACH

At first glance it may seem that finding the T-matrix is no easier than a direct solving of the Schrödinger equation (2.4). We will demonstrate, however, that the T-matrix formulation allows for a self-consistent description of the low-energy part of the spectrum that uses the *free-space* low-energy scattering properties of the interaction potential as the *only* input. In addition the low-energy (s-wave) limit is isolated to a single well-defined approximation without requiring the ad-hoc introduction of regularization via a pseudo-potential. In this section we first outline this self-consistent low-energy treatment. We then solve for the T-matrix using the standard Huang-Fermi pseudo-potential, showing that the pseudo-potential reproduces the exact result in this situation.

Let the unperturbed Hamiltonian \hat{H} be a Hamiltonian for a single nonrelativistic particle in presence of a trapping potential U :

$$\langle \mathbf{r} | \hat{H} | \psi \rangle = \left[-\frac{\hbar^2 \nabla_{\mathbf{r}}^2}{2\mu} + U(\mathbf{r}) \right] \langle \mathbf{r} | \psi \rangle, \quad (4.1)$$

Assume also that the particle is ‘perturbed’ by a scatterer given by

$$\langle \mathbf{r} | \hat{V} | \psi \rangle = V(\mathbf{r}) \langle \mathbf{r} | \psi \rangle \quad (4.2)$$

localized around $\mathbf{r} = \mathbf{0}$. In what follows we will derive a *low-energy approximation* for the T-matrix of the scatterer V in presence of \hat{H} . It is important to note that, by definition, the T-matrix acts only on eigenstates of the unperturbed Hamiltonian, which we can safely assume to be regular everywhere (this is of course a constraint on the properties of the unperturbed Hamiltonian). In this case the zero-range s-wave scattering limit does not require any regularization of the T-matrix. By making use of the Lupu-Sax formula (3.4), we first derive the correct form of the T-matrix in the low-energy s-wave regime without the introduction of a regularized pseudo-potential. In the following section, however, we will see that the results we obtain are in agreement with the standard Huang-Fermi pseudopotential approach to s-wave scattering.

We begin our derivation by first specifying a ‘reference’ background Hamiltonian \hat{H}' as

$$\langle \mathbf{r} | \hat{H}' | \psi \rangle = \left[-\frac{\hbar^2 \Delta_{\mathbf{r}}}{2\mu} + E \right] \langle \mathbf{r} | \psi \rangle. \quad (4.3)$$

This Hamiltonian is that of a free particle, but with an explicit energy dependence included so that the eigenstates have zero wavelength at all energies. We note that this reference Hamiltonian agrees with the free-space Hamiltonian in the zero-energy limit. While this Hamiltonian may seem strange, it is a valid reference Hamiltonian which turns out to be useful because the resulting T-matrix is energy independent for any scattering potential. The Green’s function for this Hamiltonian is given by

$$\langle \mathbf{r} | \hat{G}_{\hat{H}'}(E) | \mathbf{r}' \rangle = -\frac{\mu}{2\pi\hbar^2} \frac{1}{|\mathbf{r} - \mathbf{r}'|}, \quad (4.4)$$

as can be verified by direct substitution into $[E - \hat{H}'] \hat{G}_{\hat{H}'}(E) = \hat{I}$. In turn the T -matrix of the interaction potential V in presence of \hat{H}' is independent of energy and can therefore be expressed as

$$\langle \mathbf{r} | \hat{T}_{\hat{H}', \hat{V}}(E) | \mathbf{r}' \rangle = g D(\mathbf{r}, \mathbf{r}'), \quad (4.5)$$

where the kernel D is defined as normalized to unity,

$$\int d\mathbf{r} d\mathbf{r}' D(\mathbf{r}, \mathbf{r}') = 1. \quad (4.6)$$

The normalization coefficient g is then related to the 3-dimensional scattering length a according to

$$g = \frac{2\pi\hbar^2 a}{\mu}, \quad (4.7)$$

a relationship which is derived explicitly in Appendix B.4.

Imagine that the kernel $D(\mathbf{r}, \mathbf{r}')$ is well localized within some radius R . In perturbative expansions at low energies this kernel only participates in convolutions with slow (as compare to R) functions, in which case it can be approximated by a δ -function,

$$D(\mathbf{r}, \mathbf{r}') \approx \delta(\mathbf{r}) \delta(\mathbf{r}'). \quad (4.8)$$

This straightforward approximation is the key to the s-wave scattering approximation. As we demonstrate in detail in Appendix B.5, this effectively replaces the exact reference T-matrix by its long-wavelength limit, so that the reference T-matrix assumes the form

$$\langle \mathbf{r} | \hat{T}_{\hat{H}', \hat{V}}(E) | \mathbf{r}' \rangle \stackrel{k, k' \ll 1/R}{\approx} g \delta(\mathbf{r}) \delta(\mathbf{r}'), \quad (4.9)$$

which is equivalent to

$$\hat{T}_{\hat{H}', \hat{V}}(E) = g |0\rangle \langle 0|, \quad (4.10)$$

where $|0\rangle$ is the position eigenstate corresponding to the location of the scatterer. In expression (4.9) k and k' refer to the wavevectors of any matrices which multiply the T-matrix from the left and right, respectively.

If we now substitute the above expression for the reference T-matrix into the Lupu-Sax formula (3.4) for the T-matrix under the background Hamiltonian \hat{H} we arrive at

$$\begin{aligned} \hat{T}_{\hat{H}, \hat{V}}(E) &= \sum_{n=0}^{\infty} \left[g |0\rangle \langle 0| \hat{G}_{\hat{H}'}(E) \right]^n g |0\rangle \langle 0| \\ &= \left[1 - g \langle 0 | \hat{G}_{\hat{H}}(E) | 0 \rangle + g \langle 0 | \hat{G}_{\hat{H}'}(E) | 0 \rangle \right]^{-1} g |0\rangle \langle 0|. \end{aligned} \quad (4.11)$$

Making use of Eq. (4.4), we introduce the function $\chi(\mathcal{E})$, defined as

$$\chi(E) = \lim_{\mathbf{r} \rightarrow 0} \left[\langle \mathbf{r} | \hat{G}_{\hat{H}}(E) | 0 \rangle + \frac{\mu}{2\pi\hbar^2 |\mathbf{r}|} \right], \quad (4.12)$$

from which we obtain the following simple expression for the T-matrix of the scatterer \hat{V} in presence of the trap:

$$\langle \mathbf{r} | \hat{T}_{\hat{H}, \hat{V}}(E) | \psi \rangle \stackrel{E \ll \hbar^2/\mu R^2}{\approx} \frac{g \delta(\mathbf{r})}{1 - g \chi(E)} \langle \mathbf{r} | \psi \rangle. \quad (4.13)$$

As we will explicitly demonstrate for the case of transverse harmonic confinement, the singularity in bound Green's function is the same as that in the free-space Green's function. Hence, $\chi(E)$ is the value of the regular part of the bound Green's function at the origin.

5 THE FUNCTION $\chi(E)$

In this section we derive the bound Green's function of the waveguide, from which we obtain an analytic expression for regular part at the origin $\chi(E)$, which gives the energy dependence of the bound T-matrix. We begin by reviewing the eigenstates of the waveguide potential, which we then use as a basis for expanding the bound Green's function and obtaining $\chi(E)$.

5.1 Eigenstates of the waveguide Hamiltonian

The Hamiltonian for the relative motion of two atoms in a harmonic waveguide contains two parts, the longitudinal free Hamiltonian \hat{H}_z and the transverse confinement Hamiltonian \hat{H}_\perp ,

$$\hat{H} = \hat{H}_z + \hat{H}_\perp, \quad (5.1)$$

where

$$\langle \mathbf{r} | \hat{H}_z | \psi \rangle = -\frac{\hbar^2}{2\mu} \frac{\partial^2}{\partial z^2} \langle \mathbf{r} | \psi \rangle, \quad (5.2)$$

and

$$\langle \mathbf{r} | \hat{H}_\perp | \psi \rangle = \left[-\frac{\hbar^2}{2\mu} \left(\frac{\partial^2}{\partial \rho^2} + \frac{1}{\rho} \frac{\partial}{\partial \rho} + \frac{1}{\rho^2} \frac{\partial^2}{\partial \phi^2} \right) + \frac{1}{2} \mu \omega_\perp^2 \rho^2 \right] \langle \mathbf{r} | \psi \rangle. \quad (5.3)$$

The eigenstates of the transverse Hamiltonian, denoted by $|nm\rangle$, are well known and satisfy both

$$\hat{H}_\perp |n, m\rangle = \hbar \omega_\perp (2n + |m| + 1) |nm\rangle, \quad (5.4)$$

as well as

$$\hat{L}_z |nm\rangle = \hbar m |nm\rangle, \quad (5.5)$$

where \hat{L}_z is the operator for angular momentum along the z-axis. We note that in this representation the radial and azimuthal quantum numbers n and m independently assume the values

$$n = 0, 1, 2, \dots, \infty, \quad (5.6)$$

and

$$m = 0, \pm 1, \pm 2, \dots, \pm \infty. \quad (5.7)$$

The eigenfunctions are given in r-representation by

$$\langle \rho \phi | nm \rangle = \left[\frac{\pi a_\perp^2 (n + |m|)!}{n!} \right]^{-1/2} e^{-\frac{1}{2}(\rho/a_\perp)^2} (\rho/a_\perp)^{|m|} e^{im\phi} L_n^{[|m|]}(\rho^2/a_\perp^2), \quad (5.8)$$

where

$$a_\perp = \sqrt{\frac{\hbar}{\mu \omega_\perp}} \quad (5.9)$$

is the transverse harmonic oscillator length. Lastly we note that the value of $|n, m\rangle$ at the origin is given by

$$\langle 0 | nm \rangle = \frac{\delta_{m,0}}{\sqrt{\pi} a_\perp}, \quad (5.10)$$

which is independent of n .

5.2 The Green's function for the relative motion of two particles in a harmonic waveguide

The bound Green's function is the solution to the equation

$$\left[E - \hat{H}_z - \hat{H}_\perp \right] \hat{G}(E) = \hat{I}, \quad (5.11)$$

where \hat{I} is the identity matrix and for simplicity we have taken $\hat{G}_{\hat{H}}(E) \leftrightarrow \hat{G}(E)$. Expanding this equation onto the set of states

$$|nmz\rangle = |nm\rangle \otimes |z\rangle, \quad (5.12)$$

where $|nm\rangle$ is the eigenstate of \hat{H}_\perp given by (5.8) and $|z\rangle$ is the eigenstate of \hat{z} , satisfying $\langle z | z' \rangle = \delta(z - z')$, then gives

$$\begin{aligned} \left[E - \hbar \omega_\perp (2n + |m| + 1) + \frac{\hbar^2}{2\mu} \frac{\partial^2}{\partial z^2} \right] \langle nmz | \hat{G}(E) | n'm'z' \rangle &= \langle nmz | n'm'z' \rangle \\ &= \delta_{n,n'} \delta_{m,m'} \delta(z - z'). \end{aligned} \quad (5.13)$$

We proceed by making the Ansatz for the Green's function

$$\begin{aligned}\langle nmz|\hat{G}(E)|n'm'z'\rangle &= \delta_{n,n'}\delta_{m,m'}\alpha_{nm}e^{i\gamma_{nm}|z-z'|} \\ &= \delta_{n,n'}\delta_{m,m'}\alpha_{nm}\left[e^{i\gamma_{nm}(z-z')}\Theta(z-z') + e^{-i\gamma_{nm}(z-z')}\Theta(z'-z)\right],\end{aligned}\quad (5.14)$$

where $\Theta(z)$ is the Heavyside step-function. Differentiating (5.14) twice with respect to z gives

$$\frac{\partial^2}{\partial z^2}\langle nmz|\hat{G}(E)|n'm'z'\rangle = -\gamma_{nm}^2\langle nmz|\hat{G}(E)|n'm'z'\rangle + 2i\gamma_{nm}\alpha_{nm}\langle nmz|n'm'z'\rangle, \quad (5.15)$$

so the Eq. (5.13) becomes

$$\left[E - \hbar\omega_{\perp}(2n + |m| + 1) - \frac{\hbar^2\gamma_{nm}^2}{2\mu}\right]\langle nmz|\hat{G}(E)|n'm'z'\rangle + i\frac{\hbar^2\gamma_{nm}\alpha_{nm}}{\mu}\langle nmz|n'm'z'\rangle = \langle nmz|n'm'z'\rangle. \quad (5.16)$$

This equation is satisfied provided that

$$\gamma_{nm}^2 = \frac{2\mu}{\hbar^2}[E - \hbar\omega_{\perp}(2n + |m| + 1)] \quad (5.17)$$

and

$$\alpha_{nm} = -i\frac{\mu}{\hbar^2\gamma_{nm}}. \quad (5.18)$$

Equation (5.17) is quadratic, and therefore has in general two solutions. We can determine which solution is needed, however, from the causal nature of the retarded Green's function. We should choose the solutions which propagate outwards from $z = z'$.

By introducing the dimensionless energy

$$\mathcal{E} = \frac{E}{2\hbar\omega_{\perp}} - \frac{1}{2}, \quad (5.19)$$

and making use of the relation (5.9), we find that retarded Green's function can be expressed as

$$\langle nmz|\hat{G}(\mathcal{E})|n'm'z'\rangle = -i\frac{\mu a_{\perp}}{2\hbar^2}\frac{e^{i\frac{2}{a_{\perp}}\sqrt{\mathcal{E}-n-\frac{|m|}{2}}|z-z'|}}{\sqrt{\mathcal{E}-n-\frac{|m|}{2}}}\delta_{n,n'}\delta_{m,m'}. \quad (5.20)$$

With this expression for the bound Green's function we can now proceed to compute the bound T-matrix via equation (4.13).

5.3 The function $\chi(\mathcal{E})$ for a point scatterer in presence of a wave-guide

In order to evaluate $\chi(\mathcal{E})$ we must first compute the matrix element $\langle \mathbf{r}|\hat{G}(\mathcal{E})|0\rangle$. Expanding this matrix element in terms of transverse eigenstates gives

$$\langle \mathbf{r}|\hat{G}(\mathcal{E})|0\rangle = \sum_{nmn'm'} \langle \rho\phi|nm\rangle \langle nmz|\hat{G}(\mathcal{E})|n'm'0\rangle \langle n'm'0|0\rangle, \quad (5.21)$$

which, with the help of Eqs. (5.10) and (5.20), gives

$$g\langle \mathbf{r}|\hat{G}(\mathcal{E})|0\rangle = -\sqrt{\pi}a \sum_{n=0}^{\infty} \langle \rho\phi|n0\rangle \frac{e^{-\frac{2}{a_{\perp}}\sqrt{n-\mathcal{E}}|z|}}{\sqrt{n-\mathcal{E}}}, \quad (5.22)$$

where the modified square root $\sqrt[n]{\cdot}$ is defined in the “Conventions and notations” table above. Now by inserting Eqs. (5.22) and (4.7) into Eq. (4.12) we arrive at the expression

$$g\chi(\mathcal{E}) = \lim_{\mathbf{r} \rightarrow 0} \left[-\sqrt{\pi}a \sum_{n=0}^{\infty} \langle \rho\phi | n0 \rangle \frac{e^{-\frac{2}{a_{\perp}} \sqrt[n]{n-\mathcal{E}}|z|}}{\sqrt[n]{n-\mathcal{E}}} + \frac{a}{|\mathbf{r}|} \right]. \quad (5.23)$$

While both terms in Eq. (5.23) diverge in the limit $\mathbf{r} \rightarrow \infty$, we now demonstrate that their difference remains finite and leads to an expression for $\chi(\mathcal{E})$ in terms of a generalized Zeta function.

First we assume, without a proof, that the multi-variable limit in Eq. (5.23) does exist, *i.e.* the directional single-variable limits $\mathbf{r} = s\mathbf{n}$, $s \rightarrow 0$ exist for all directions \mathbf{n} and they are all equal to each other. This assumption allows us to deal with the limit along the z-axis only:

$$g\chi(\mathcal{E}) = -\frac{a}{a_{\perp}} \lim_{|z| \rightarrow 0} \left[\sum_{n=0}^{\infty} \frac{e^{-\frac{2}{a_{\perp}} \sqrt[n]{n-\mathcal{E}}|z|}}{\sqrt[n]{n-\mathcal{E}}} - \frac{a}{|z|} \right], \quad (5.24)$$

where we have used the identity (5.10). We proceed by first replacing the $a/|\mathbf{r}|$ term in Eq. (5.24) with an integral expression via the identity

$$\frac{a}{|\mathbf{r}|} = \frac{a}{a_{\perp}} \int_{\mathcal{E}}^{\infty} dn \frac{e^{-\frac{2}{a_{\perp}} \sqrt{n-\mathcal{E}}|\mathbf{r}|}}{\sqrt{x-\mathcal{E}}}. \quad (5.25)$$

This allows us to write

$$g\chi(\mathcal{E}) = -\frac{a}{a_{\perp}} \lim_{|z| \rightarrow 0} \lim_{N \rightarrow \infty} \left[\sum_{n=0}^N \frac{e^{-\frac{2}{a_{\perp}} \sqrt[n]{n-\mathcal{E}}|z|}}{\sqrt[n]{n-\mathcal{E}}} - \int_{\mathcal{E}}^N dn \frac{e^{-\frac{2}{a_{\perp}} \sqrt{n-\mathcal{E}}|\mathbf{r}|}}{\sqrt{n-\mathcal{E}}} \right], \quad (5.26)$$

It is now tempting to interchange the limit signs and thus get rid of the coordinate dependence. In order to be able to do that one have to prove the uniformity with respect to $|z|$ of the $N \rightarrow \infty$ convergence of the expression in the square brackets $\Xi(N, |z|)$, *i.e.* to prove that for every ϵ there exists N^* , the same for all $|z|$, such that $\Xi(N, |z|) - \lim_{N \rightarrow \infty} \Xi(N, |z|) < \epsilon$ for all $N > N^*$. Such a proof does exist: provided its length we do not exhibit it here.

We arrive at the following expression for $\chi(\mathcal{E})$:

$$g\chi(\mathcal{E}) = -\frac{a}{a_{\perp}} \lim_{N \rightarrow \infty} \left[\sum_{n=0}^N \frac{1}{\sqrt[n]{n-\mathcal{E}}} - 2\sqrt{N-\mathcal{E}} \right]. \quad (5.27)$$

One can now make use of the following theorem involving the Hurwitz Zeta function, an analytic generalized Zeta function described in the mathematical literature [6],

$$\zeta(s, \alpha) = \lim_{N \rightarrow \infty} \left[\left(\sum_{n=0}^N \frac{1}{(n+\alpha)^s} \right) - \frac{1}{1-s} \frac{1}{(N+\alpha)^{s-1}} \right] \quad (5.28)$$

$\text{Re}(s) > 0, \quad -2\pi < \arg(n+\alpha) \leq 0.$

In particular,

$$\zeta(1/2, \alpha) = \lim_{N \rightarrow \infty} \left[\left(\sum_{n=0}^N \frac{1}{\sqrt[n]{n+\alpha}} \right) - 2\sqrt{N+\alpha} \right]. \quad (5.29)$$

While this expression, valid for any N , may be taken as a definition of the Hurwitz Zeta function, it does not constitute an efficient method for computation. Most symbolic math software packages will have efficient algorithms, however in using them care must be taken with regards to the branch cut for fractional s . With this definition and taking $s = 1/2$ we arrive at

$$g\chi(\mathcal{E}) = -\frac{a}{a_{\perp}}\zeta(1/2, -\mathcal{E}). \quad (5.30)$$

By substituting this expression into Eq. (4.13) we arrive at the final expression for the long-wavelength T-matrix in the waveguide:

$$\hat{T}(\mathcal{E}) = \frac{g|0\rangle\langle 0|}{1 + \frac{a}{a_{\perp}}\zeta(1/2, -\mathcal{E})}. \quad (5.31)$$

We note that in the definition (5.28) of the Hurwitz Zeta function, there is an ambiguity in the sign of the square root.

6 RESULTS

6.1 Multi-channel scattering amplitudes and transition rates

From Equations (3.8) and (5.31) we find that the scattered wavefunction takes the form

$$\langle nmz|\psi_s(\mathcal{E})\rangle = g \frac{\langle nmz|\hat{G}(\mathcal{E})|0\rangle}{\left[1 + \frac{a}{a_{\perp}}\zeta(1/2, -\mathcal{E})\right]} \langle 0|\psi_0(\mathcal{E})\rangle. \quad (6.1)$$

Now the matrix element $\langle nmz|\hat{G}(\mathcal{E})|0\rangle$ can be determined by making use of Eqs. (5.20) and (5.10), yielding

$$\begin{aligned} \langle nmz|\hat{G}(\mathcal{E})|0\rangle &= \sum_{n'm'} \int dz' \langle nmz|\hat{G}(\mathcal{E})|n'm'z'\rangle \langle n'm'z'|0\rangle \\ &= -i \frac{\mu}{2\sqrt{\pi}\hbar^2} \delta_{m,0} \frac{e^{i\frac{2}{a_{\perp}}\sqrt{\mathcal{E}-n}|z|}}{\sqrt{\mathcal{E}-n}}. \end{aligned} \quad (6.2)$$

Inserting this expression into Eq. (6.1) then gives

$$\langle nmz|\psi_s(\mathcal{E})\rangle = -i \frac{\sqrt{\pi}a}{\left[1 + \frac{a}{a_{\perp}}\zeta(1/2, -\mathcal{E})\right]} \delta_{m,0} \frac{e^{i\frac{2}{a_{\perp}}\sqrt{\mathcal{E}-n}|z|}}{\sqrt{\mathcal{E}-n}} \langle 0|\psi_0(\mathcal{E})\rangle. \quad (6.3)$$

Let us now assume that the incident wave has the longitudinal wave vector k and the transverse quantum numbers n and m , according to

$$\langle \mathbf{r}|\psi_0(\mathcal{E})\rangle = \langle \rho\phi|nm\rangle e^{ikz}, \quad (6.4)$$

where the relation

$$\mathcal{E} = \left(\frac{a_{\perp}k}{2}\right)^2 + n + \frac{|m|}{2} \quad (6.5)$$

gives the dependence of the scaled energy \mathcal{E} on the incident wavevector k . This incident wave is nonzero at the origin only for $m = 0$, hence only incident waves with zero angular

momentum will scatter. The value of the $m = 0$ incident wave at the origin conveniently takes the n -independent value,

$$\langle 0|\psi_0(\mathcal{E})\rangle = \frac{\delta_{m,0}}{\sqrt{\pi}a_{\perp}}. \quad (6.6)$$

Assuming henceforth $m = 0$, we can now express Eq. (6.3) as

$$\langle n'm'z|\psi_s(\mathcal{E})\rangle = -i \frac{\delta_{m',0}}{\left[\frac{a_{\perp}}{a} + \zeta(1/2, -\mathcal{E})\right]} \frac{e^{i\frac{2}{a_{\perp}}\sqrt{\mathcal{E}-n'}|z|}}{\sqrt{\mathcal{E}-n'}}. \quad (6.7)$$

From this expression it follows that the full wavefunction of the relative motion takes the form

$$\langle \mathbf{r}|\psi(\mathcal{E})\rangle = \sum_{n'=0}^{\infty} \langle \rho\phi|n'0\rangle \left[\delta_{n',n} e^{ikz} + f(k_{n'} \leftarrow k_n)_{n' \leftarrow n} e^{ik_{n'}|z|} \right]. \quad (6.8)$$

Here we have introduced the even-wave *transversely inelastic scattering amplitudes* $f(k_{n'} \leftarrow k_n)_{n' \leftarrow n}$, given by

$$f(k_{n'} \leftarrow k_n)_{n' \leftarrow n} = -\frac{2i}{a_{\perp}k_{n'}} \frac{1}{\left[\frac{a_{\perp}}{a} + \zeta(1/2, -\left(\frac{a_{\perp}k_n}{2}\right)^2 - n\right]}, \quad (6.9)$$

and the outgoing wave vector for the mode $|n'0\rangle$

$$k_{n'} = \frac{2}{a_{\perp}} \sqrt{\left(\frac{a_{\perp}k_n}{2}\right)^2 + n - n'}, \quad (6.10)$$

from which the desired scattering probabilities can be computed.

One can now easily compute the elastic and inelastic transition probabilities for collisions under transverse harmonic confinement. We begin by considering the asymptotic forms of the total wavefunction given by Eq. (6.8), which are given by

$$\lim_{z \rightarrow \infty} \langle n'0z|\psi(\mathcal{E})\rangle = \delta_{n',n} e^{ikz} + \Theta[\mathcal{E} - n'] f(k_{n'} \leftarrow k_n)_{n' \leftarrow n} e^{ik_{n'}z} \quad (6.11)$$

$$\lim_{z \rightarrow -\infty} \langle n0z|\psi(\mathcal{E})\rangle = \Theta[\mathcal{E} - n'] f(k_{n'} \leftarrow k_n)_{n' \leftarrow n} e^{-ik_{n'}z}. \quad (6.12)$$

Because of energy conservation, an inelastic collision results in a change in the longitudinal momentum $k \rightarrow k_n$, so that the introduction of inelastic transmission and reflection coefficients must be based on conservation of total incident and outgoing probability current. For longitudinal plane waves the probability current is given by the amplitude squared times the velocity, which leads to the inelastic transmission and reflection coefficients

$$T(k_{n'} \leftarrow k_n)_{n' \leftarrow n} = \Theta[\mathcal{E} - n'] \sqrt{\frac{\mathcal{E} - n'}{\mathcal{E} - n}} |\delta_{n',n} + f(k_{n'} \leftarrow k_n)_{n' \leftarrow n}|^2 \quad (6.13)$$

$$R(k_{n'} \leftarrow k_n)_{n' \leftarrow n} = \Theta[\mathcal{E} - n'] \sqrt{\frac{\mathcal{E} - n'}{\mathcal{E} - n}} |f(k_{n'} \leftarrow k_n)_{n' \leftarrow n}|^2, \quad (6.14)$$

which are readily evaluated with the help of Eq. (6.9). The sum of the transmission and reflection coefficients of the particular channel gives the corresponding transition probability governing the population exchange between the transverse vibrational levels.

Substituting the expression (6.9) to the transmission and reflection coefficients above we obtain the following set of kinetic coefficients:

$$W_{\leftrightarrow n}(k) = 1 - W_{\leftarrow n}(k) \quad (6.15)$$

$$W_{\leftarrow n}(k) = \frac{2}{\sqrt{\mathcal{E}_t}} \frac{\eta(\mathcal{E}) - 1/\sqrt{\mathcal{E}_t}}{[\frac{a}{a_\perp} + \zeta(1/2, 1 - \delta\mathcal{E})]^2 + \eta^2(\mathcal{E})} \quad (6.16)$$

$$W_{n' \leftarrow n}(k) = \Theta[\mathcal{E} - n'] \frac{2}{\sqrt{\mathcal{E}_t}} \frac{1}{\sqrt{\mathcal{E} - n'}} \frac{1}{[\frac{a}{a_\perp} + \zeta(1/2, 1 - \delta\mathcal{E})]^2 + \eta^2(\mathcal{E})} \quad (6.17)$$

$$T_{\leftrightarrow n}(k) = W_{\leftrightarrow n}(k) - R_{\leftrightarrow n}(k) \quad (6.18)$$

$$R_{\leftrightarrow n}(k) = \frac{1}{\mathcal{E}_t} \frac{1}{[\frac{a}{a_\perp} + \zeta(1/2, 1 - \delta\mathcal{E})]^2 + \eta^2(\mathcal{E})} \quad (6.19)$$

$$T_{n' \leftarrow n}(k) = R_{n' \leftarrow n}(k) = W_{n' \leftarrow n}(k)/2 \quad (6.20)$$

where $W_{\leftrightarrow n}(k)$ is the probability that after a collision of two particles with the relative momentum k and relative transverse excitation n the particles will remain in the same transverse state, this probability is a sum of transmission $T_{\leftrightarrow n}(k)$ and reflection $R_{\leftrightarrow n}(k)$ probabilities, $W_{\leftarrow n}(k)$ is the total probability of changing the transverse state, $W_{n' \leftarrow n}(k)$ is the probability of transition to a particular transverse channel, the transmission $T_{n' \leftarrow n}(k)$ and reflection $R_{n' \leftarrow n}(k)$ probabilities in channel-changing collisions are equal to each other. Here

$$\mathcal{E} = n + \mathcal{E}_t \quad (6.21)$$

$$\mathcal{E}_t = (ka_\perp/2)^2 \quad (6.22)$$

$$\delta\mathcal{E} = \mathcal{E} - [\mathcal{E}] \quad 0 \leq \delta\mathcal{E} < 1 \quad (6.23)$$

$$\eta(\mathcal{E}) = \sum_{n'=0}^{[\mathcal{E}]} \frac{1}{\sqrt{\mathcal{E} - n'}} \quad (6.24)$$

where $[\dots]$ is the integral part sign.

6.2 Single-channel scattering and effective one-dimensional interaction potential

Let us now consider the special case of a single-channel scattering:

$$0 \leq \mathcal{E} < 1, \quad n_0 = 0 \quad (6.25)$$

In this case we have

$$g\chi(\mathcal{E}) = -\frac{a}{a_\perp} \zeta(1/2, -\mathcal{E}) = -\frac{a}{a_\perp} \left[\zeta(1/2, 1 - \mathcal{E}) + \frac{i}{\sqrt{\mathcal{E}}} \right]. \quad (6.26)$$

Using an alternative representation for $\zeta(1/2, 1 - \mathcal{E})$

$$\zeta(1/2, 1 - \mathcal{E}) = \lim_{N \rightarrow \infty} \left[\sum_{n=1}^N \frac{1}{\sqrt{n - \mathcal{E}}} - 2\sqrt{N} \right]. \quad (6.27)$$

and making use of the expansion in powers of \mathcal{E} ,

$$\frac{1}{\sqrt{n - \mathcal{E}}} = \frac{1}{\sqrt{n}} + \sum_{j=1}^{\infty} \frac{(2j-1)!!}{2^j j! n^{j+1/2}} \mathcal{E}^j \quad (6.28)$$

$$|\mathcal{E}| < 1, \quad n > 0,$$

allows us to write

$$\zeta(1/2, 1 - \mathcal{E}) = \zeta(1/2) + \mathcal{L}(\mathcal{E}), \quad (6.29)$$

where

$$\mathcal{L}(\mathcal{E}) = \sum_{j=1}^{\infty} \frac{(2j-1)!! \zeta(j+1/2)}{2^j j!} \mathcal{E}^j, \quad (6.30)$$

which clearly separates the zero energy limit from the finite energy corrections.

According to (6.9) this leads to

$$f_e(k) = -\frac{1}{\left[1 + ia_{1D}k - i\frac{a_{\perp}k}{2} \mathcal{L}\left(\frac{a_{\perp}^2 k^2}{4}\right)\right]}, \quad (6.31)$$

where $f_e(k) = f(k_0 \leftarrow k_0)_{0 \leftarrow 0}$ is the even single-channel scattering amplitude and

$$a_{1D} = -\frac{a_{\perp}}{2} \left[\frac{a_{\perp}}{a} + \zeta(1/2) \right] \quad (6.32)$$

with $\zeta(1/2) = -1.4603\dots$, is the effective one-dimensional scattering length which agrees with the result in [1].

It is now tempting to introduce an effective one-dimensional interaction potential in such a way that its scattering amplitude, introduced through the one-dimensional scattering solution as

$$\psi(z) \stackrel{z \rightarrow \pm\infty}{\sim} \exp(ikz) + f_e(k) \exp(ik|z|) + f_o(k) \text{sign}(z) \exp(ik|z|) \quad , \quad (6.33)$$

matches (6.31), i.e. solve the corresponding one-dimensional inverse scattering problem. It turns out that this problem is ill-posed due to the presence of open transverse channels inaccessible within the one-dimensional model. Nevertheless one may pose the following problem: find a one-dimensional potential, whose scattering amplitude reproduces the exact one (6.31) with the relative error $\mathcal{O}(k^3)$. Such an object does exist, and it is represented by a zero-range scatterer

$$v(z) = g_{1D} \delta(z) \quad (6.34)$$

of a coupling strength $g_{1D} = -\hbar^2/\mu a_{1D}$.

Notice now the resonant behavior of g_{1D} showing a Confinement Induced Resonance (CIR) at $a = a_{\perp}/|\zeta(1/2)|$. The effect was recently interpreted in terms of Feshbach resonance between ground and excited vibrational manifolds. The resonance has been confirmed by numerical calculations with finite-range potentials, at both two-body [2] and many-body [7] level.

6.3 Bound states

As it has been discussed in the section 3.3 the poles of the full T-matrix of the problem (the T-matrix 5.31 in our case) correspond to the bound states. We get the following eigenvalue equation

$$\zeta(1/2, -\mathcal{E}) = -\frac{a_{\perp}}{a} \quad (6.35)$$

The detailed analysis, interpretation, and testing of the solutions against finite-range models is presented in [2]. It turns out that for any set of parameters there exists one and only one bound state. For small positive three-dimensional scattering length it converges to the free-space three-dimensional bound state. For small negative scattering length the bound state corresponds to the bound state of the one-dimensional potential (6.34).

7 CONCLUDING REMARKS, RELATED WORKS, AND OPEN PROBLEMS

In this paper we have demonstrated that the low-energy free-space properties of a scatterer are sufficient to describe its low-energy behavior in a non-free environment. The T-matrix formalism and the Lupu-Sax connection formula in particular serve as a powerful bridge between the two.

Several related works ought to be mentioned. Scattering of bosons in two-dimensional (planar) harmonic waveguides has been successfully treated in [3]. Fermions in a linear guide were considered in [4] via the K-matrix formalism and the corresponding one-dimensional amplitudes were explicitly computed. In an N -body setting $N - 2$ particles can be interpreted as the background potential for a given pair [8].

One would expect that the inverse scattering problem posed in section 6.2 can be solved with an accuracy higher than existing $\mathcal{O}(k^3)$. The solution will allow to improve the accuracy of the many-body Monte-Carlo numerical models without introducing the transverse dimensions, otherwise making the computation harder.

Shallow atomic guides with only a few transverse bound levels constitute a significant challenge. Unlike for harmonic guides the separation of relative and transverse degrees of freedom will be lifted leading to new collision channels. Presence of continuum spectrum for virtual transverse excitations may significantly enhance the renormalization effects or even lead to new resonances.

APPENDIX

A ACKNOWLEDGMENTS

Authors are grateful to Adam Lupu-Sax, Rick Heller, Vanja Dunjko, Yvan Castin, and Dmitry Petrov for enlightening discussions on the subject. This work was supported by the National Science Foundation grant *PHY-0070333* (M.O.), a grant from Office of Naval Research *N00014-03-1-0427* (T.B., M.O.), and through the National Science Foundation grant for the Institute for Theoretical Atomic and Molecular Physics at Harvard University and Smithsonian Astrophysical Observatory.

B APPENDICES

B.1 The T-matrix, the potential and the background Green's function

In this section we derive various useful relationships between the Green's function of a given background Hamiltonian, $\hat{G}_{\hat{H}}(E)$, the scattering potential, \hat{V} , and the T-matrix, $\hat{T}_{\hat{H},\hat{V}}(E)$, which connects the incident wavevector $|\psi_0(E)\rangle$ with the scattered wave $|\psi_s(E)\rangle$ according to Eq. (3.8). By making use of the definition of the T-matrix (3.8) and the fact that the incident wave satisfies the unperturbed Hamiltonian (3.6), we can cast Schrödinger's equation (3.7) in the following form

$$\left[\hat{T}_{\hat{H},\hat{V}}(E) - \hat{V} \hat{G}_{\hat{H}}(E) \hat{T}_{\hat{H},\hat{V}}(E) - \hat{V} \right] |\psi_0(E)\rangle. \quad (\text{B.1})$$

Since this equation must be satisfied for any $|\psi_0(E)\rangle$ it follows that

$$\hat{T}_{\hat{H},\hat{V}}(E) - \hat{V} \hat{G}_{\hat{H}}(E) \hat{T}_{\hat{H},\hat{V}}(E) - \hat{V} = 0. \quad (\text{B.2})$$

This equation can be readily solved for either the T-matrix $\hat{T}_{\hat{H},\hat{V}}(E)$ or the potential \hat{V} . Solving first for $\hat{T}_{\hat{H},\hat{V}}(E)$ then gives

$$\hat{T}_{\hat{H},\hat{V}}(E) = \left[1 - \hat{V}\hat{G}_{\hat{H}}(E)\right]^{-1} \hat{V}, \quad (\text{B.3})$$

which gives an expression for the T-matrix at energy E in terms of the perturbation \hat{V} and the background Green's function $\hat{G}_{\hat{H}}(E)$. We can also solve Eq. (B.2) for \hat{V} , which yields

$$\hat{V} = \hat{T}_{\hat{H},\hat{V}}(E) \left[1 + \hat{G}_{\hat{H}}(E)\hat{T}_{\hat{H},\hat{V}}(E)\right]^{-1}, \quad (\text{B.4})$$

or by starting from the Hermite conjugate of Eq. (3.7) we can similarly arrive at the equivalent expression

$$\hat{V} = \left[1 + \hat{T}_{\hat{H},\hat{V}}(E)\hat{G}_{\hat{H}}(E)\right]^{-1} \hat{T}_{\hat{H},\hat{V}}(E). \quad (\text{B.5})$$

B.2 The Lippman-Schwinger equation

In this section we derive the relation between the full Green's function of the Hamiltonian $\hat{H} + \hat{V}$ in terms of the Green's function for the Hamiltonian \hat{H} and the T-matrix. The full Green's function can be defined by

$$\hat{G}_{\hat{H}+\hat{V}}^{-1}(E) = \hat{G}_{\hat{H}}^{-1} - \hat{V}, \quad (\text{B.6})$$

which, after substituting Eq. (B.4) yields

$$\hat{G}_{\hat{H}+\hat{V}}^{-1}(E) = \hat{G}_{\hat{H}}^{-1} - \hat{T}_{\hat{H},\hat{V}}(E) \left[1 + \hat{G}_{\hat{H}}(E)\hat{T}_{\hat{H},\hat{V}}(E)\right]^{-1}. \quad (\text{B.7})$$

Multiplying from the left by $\hat{G}_{\hat{H}+\hat{V}}(E)$ and then from the right by $\left[1 + \hat{G}_{\hat{H}}(E)\hat{T}_{\hat{H},\hat{V}}(E)\right] \hat{G}_{\hat{H}}(E)$ then yields the Lippman-Schwinger relation

$$\hat{G}_{\hat{H}+\hat{V}}(E) = \hat{G}_{\hat{H}}(E) + \hat{G}_{\hat{H}}(E)\hat{T}_{\hat{H},\hat{V}}(E)\hat{G}_{\hat{H}}(E) \quad (\text{B.8})$$

which relates the full Green's function to the 'background' Green's function and T-matrix.

B.3 The Lupu-Sax formula

In many situations one may not have knowledge of the potential \hat{V} , but rather have direct knowledge only of the T-matrix, $\hat{T}_{\hat{H}',\hat{V}}(E)$ with respect to some background Hamiltonian \hat{H}' . If additional external fields are applied, then ideally one would like an expression for the T-matrix of the same perturbation in the presence the new background Hamiltonian $\hat{T}_{\hat{H},\hat{V}}(E)$.

We can derive the required expression directly from the relations (B.4) and (B.5). Since \hat{V} is equal to itself we can equate expression (B.4) for \hat{V} in terms of \hat{H}' to the equivalent expression (B.5) in terms of \hat{H} , which yields the relation

$$\left[1 + \hat{T}_{\hat{H}',\hat{V}}(E)\hat{G}_{\hat{H}'}(E)\right]^{-1} \hat{T}_{\hat{H}',\hat{V}}(E) = \hat{T}_{\hat{H},\hat{V}}(E) \left[1 + \hat{G}_{\hat{H}}(E)\hat{T}_{\hat{H},\hat{V}}(E)\right]^{-1}. \quad (\text{B.9})$$

Multiplying from the left by $1 + \hat{T}_{\hat{H}',\hat{V}}(E)\hat{G}_{\hat{H}'}(E)$ and from the right by $1 + \hat{G}_{\hat{H}}(E)\hat{T}_{\hat{H},\hat{V}}(E)$ then gives

$$\hat{T}_{\hat{H},\hat{V}}(E) \left[1 + \hat{G}_{\hat{H}}(E)\hat{T}_{\hat{H},\hat{V}}(E)\right] = \left[1 + \hat{T}_{\hat{H}',\hat{V}}(E)\hat{G}_{\hat{H}'}(E)\right] \hat{T}_{\hat{H},\hat{V}}(E). \quad (\text{B.10})$$

We note that in this equation the unknown operator $\hat{T}_{\hat{H},\hat{V}}(E)$ appears linearly and always on the far-right side. Hence, solving for $\hat{T}_{\hat{H},\hat{V}}(E)$ is straightforward and results in the Lupu-Sax formula [5] relating the T -matrices of the same perturbation but in two different background Hamiltonians \hat{H} and \hat{H}' :

$$\hat{T}_{\hat{H},\hat{V}}(E) = \left[1 - \hat{T}_{\hat{H}',\hat{V}}(E) \left(\hat{G}_{\hat{H}}(E) - \hat{G}_{\hat{H}'}(E) \right) \right]^{-1} \hat{T}_{\hat{H}',\hat{V}}(E). \quad (\text{B.11})$$

B.4 The free-space scattering length

In this section we will relate the 3-dimensional scattering length to the normalization of the kernel of the reference T-matrix (4.5). In Section 4 we introduced the reference Hamiltonian $\hat{H}' = \hat{H}_{free} + E$, where \hat{H}_{free} is the free-space Hamiltonian containing only a 3-dimensional kinetic energy term. We note that for $E = 0$ the reference Hamiltonian and the free-space Hamiltonian agree, hence we can use the Green's function and T-matrix of \hat{H}' to solve the free-space scattering problem at zero energy. The free-space solution for scattering from the potential \hat{V} is therefore given at $E = 0$ by

$$|\psi_s(0)\rangle = \hat{G}_{\hat{H}'}(0) \hat{T}_{\hat{H}',\hat{V}}(0) |\psi_0(0)\rangle \quad (\text{B.12})$$

where $\hat{G}_{\hat{H}'}(0)$ is given by Eq. (4.4) and $\hat{T}_{\hat{H}',\hat{V}}(0)$ by Eq. (4.5). Expanding this expression onto position eigenstates and making use of (4.4) and (4.5) gives

$$\langle \mathbf{r} | \psi_s(0) \rangle = -\frac{\mu g}{2\pi\hbar^2} \int d\mathbf{r}' d\mathbf{r}'' \frac{D(\mathbf{r}', \mathbf{r}'')}{|\mathbf{r} - \mathbf{r}'|} \langle \mathbf{r}'' | \psi_0(0) \rangle. \quad (\text{B.13})$$

For zero energy the incident wave is given by $\langle \mathbf{r} | \psi_0(0) \rangle = 1$, hence by making the assumption that $D(\mathbf{r}', \mathbf{r}'')$ is localized at $\mathbf{r}', \mathbf{r}'' \approx 0$ we find that the limit as $\mathbf{r} \rightarrow \infty$ is given by

$$\begin{aligned} \lim_{\mathbf{r} \rightarrow \infty} \langle \mathbf{r} | \psi_s(0) \rangle &= -\frac{\mu g}{2\pi\hbar^2} \frac{1}{|\mathbf{r}|} \int d\mathbf{r}' d\mathbf{r}'' D(\mathbf{r}', \mathbf{r}'') \\ &= -\frac{\mu g}{2\pi\hbar^2} \frac{1}{|\mathbf{r}|}. \end{aligned} \quad (\text{B.14})$$

Because the potential is assumed to vanish as $\mathbf{r} \rightarrow \infty$, we know that the asymptotic form of the scattered wavefunction is given by a spherical plane wave with zero kinetic energy, characterized by the zero-energy scattering amplitude $f_s(0)$,

$$\lim_{\mathbf{r} \rightarrow \infty} \langle \mathbf{r} | \psi_s(0) \rangle = f_s(0) \frac{1}{|\mathbf{r}|}. \quad (\text{B.15})$$

Comparison with Eq. (B.14) then shows that the zero-energy scattering amplitude is

$$f_s(E=0) = -\frac{\mu g}{2\pi\hbar^2}. \quad (\text{B.16})$$

The asymptotic form of the total wavefunction is then

$$\lim_{\mathbf{r} \rightarrow \infty} \langle \mathbf{r} | \psi(0) \rangle = 1 - \frac{\mu g}{2\pi\hbar^2} \frac{1}{|\mathbf{r}|}. \quad (\text{B.17})$$

By definition, the scattering length is the radius of the first node of wavefunction at zero energy. Setting Eq. (B.17) equal to zero and solving for \mathbf{r} then gives

$$a = \frac{\mu g}{2\pi\hbar^2}, \quad (\text{B.18})$$

which relates the scattering length a and the normalization of the reference T-matrix, giving the standard expression $g = 2\pi\hbar^2 a / \mu$.

B.5 The s-wave scattering approximation

In this section we will discuss the long-wavelength properties of the reference T-matrix (4.5) and motivate the s-wave scattering approximation in which we replace this T-matrix by its long-wavelength (low energy) limit. From Eq. (4.5) we have

$$\langle \mathbf{r} | \hat{T}_{\hat{H}', \hat{V}} | \mathbf{r}' \rangle = g D(\mathbf{r}, \mathbf{r}'), \quad (\text{B.19})$$

where the kernel $D(\mathbf{r}, \mathbf{r}')$ is defined as normalized to unity. We note that the exact expression for $D(\mathbf{r}, \mathbf{r}')$ via Eqs. (3.2) and (4.4) is given by

$$\begin{aligned} g D(\mathbf{r}, \mathbf{r}') &= V(\mathbf{r}) \delta(\mathbf{r} - \mathbf{r}') + \left[\frac{-\mu}{2\pi\hbar^2} \right] \frac{V(\mathbf{r})V(\mathbf{r}')}{|\mathbf{r} - \mathbf{r}'|} + \left[\frac{-\mu}{2\pi\hbar^2} \right]^2 V(\mathbf{r})V(\mathbf{r}') \int d\mathbf{r}'' \frac{V(\mathbf{r}'')}{|\mathbf{r} - \mathbf{r}''||\mathbf{r}'' - \mathbf{r}'|} \\ &+ \left[\frac{-\mu}{2\pi\hbar^2} \right]^3 V(\mathbf{r})V(\mathbf{r}') \int d\mathbf{r}'' d\mathbf{r}''' \frac{V(\mathbf{r}'')V(\mathbf{r}''')}{|\mathbf{r} - \mathbf{r}''||\mathbf{r}'' - \mathbf{r}'''||\mathbf{r}''' - \mathbf{r}'|} + \dots, \end{aligned} \quad (\text{B.20})$$

from which we see that $D(\mathbf{r}', \mathbf{r}) = D(\mathbf{r}, \mathbf{r}')$. We will make use of these expressions in what follows.

At present we are interested in the long-wavelength (low energy) properties of this reference T-matrix, hence we begin by expanding (B.19) onto momentum eigenstates, yielding

$$\langle \mathbf{k} | \hat{T}_{\hat{H}', \hat{V}} | \mathbf{k}' \rangle = \frac{g}{(2\pi)^3} \int d\mathbf{r} d\mathbf{r}' e^{-i\mathbf{k}\cdot\mathbf{r}} e^{i\mathbf{k}'\cdot\mathbf{r}'} D(\mathbf{r}, \mathbf{r}'). \quad (\text{B.21})$$

By applying the gradient operators $\nabla_{\mathbf{k}}$ and $\nabla'_{\mathbf{k}}$ we see that

$$\begin{aligned} \nabla_{\mathbf{k}} \langle \mathbf{k} | \hat{T}_{\hat{H}', \hat{V}} | \mathbf{k}' \rangle \big|_{\mathbf{k}, \mathbf{k}'=0} &= -i \frac{g}{(2\pi)^3} \int d\mathbf{r} d\mathbf{r}' \mathbf{r} D(\mathbf{r}, \mathbf{r}') \\ &= -\nabla_{\mathbf{k}'} \langle \mathbf{k} | \hat{T}_{\hat{H}', \hat{V}} | \mathbf{k}' \rangle \big|_{\mathbf{k}, \mathbf{k}'=0}. \end{aligned} \quad (\text{B.22})$$

From Eq. (B.20) we see that $\int d\mathbf{r}' D(\mathbf{r}, \mathbf{r}')$ is an even function of \mathbf{r} provided only that $V(-\mathbf{r}) = V(\mathbf{r})$. Hence the r.h.s of Eq. (B.22) is the integral of an odd function which leads to

$$\nabla_{\mathbf{k}} \langle \mathbf{k} | \hat{T}_{\hat{H}', \hat{V}} | \mathbf{k}' \rangle \big|_{\mathbf{k}, \mathbf{k}'=0} = \nabla_{\mathbf{k}'} \langle \mathbf{k} | \hat{T}_{\hat{H}', \hat{V}} | \mathbf{k}' \rangle \big|_{\mathbf{k}, \mathbf{k}'=0} = 0. \quad (\text{B.23})$$

The fact that the gradient vanishes at $\mathbf{k}, \mathbf{k}' = 0$ implies that this point is either an extremum or inflection point, i.e. the reference T-matrix is topologically flat in the long wavelength limit. Extending this approach will lead to the result that the curvature in k-space is proportional to the second moment of $D(\mathbf{r}, \mathbf{r}')$ so that we can approximate the T-matrix by its long-wavelength limit provided that $|\mathbf{k}|R \approx |\mathbf{k}'|R \ll 1$, where R is roughly the radius of the kernel $D(\mathbf{r}, \mathbf{r}')$. Replacing the reference T-matrix by its long-wavelength limit and recalling that the kernel is normalized to unity gives

$$\langle \mathbf{k} | \hat{T}_{\hat{H}', \hat{V}} | \mathbf{k}' \rangle \approx \frac{g}{(2\pi)^3}, \quad (\text{B.24})$$

which then leads to the delta-function approximation

$$\begin{aligned} \langle \mathbf{r} | \hat{T}_{\hat{H}', \hat{V}} | \mathbf{r}' \rangle &\approx \frac{g}{(2\pi)^6} \int d\mathbf{k} d\mathbf{k}' e^{i\mathbf{k}\cdot\mathbf{r}} e^{-i\mathbf{k}'\cdot\mathbf{r}'} \\ &= g \delta(\mathbf{r}) \delta(\mathbf{r}') \end{aligned} \quad (\text{B.25})$$

which is the main result of this section.

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